Confinement vs Deconfinement of Cooper Pairs in One-Dimensional Spin-3/2 Fermionic Cold Atoms

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The phase diagram of spin-3/2 fermionic cold atoms trapped in a one-dimensional optical lattice is investigated at quarter filling (one atom per site) by means of large-scale numerical simulations. In full agreement with a recent low-energy approach, we find two phases with confined and deconfined Cooper pairs separated by an Ising quantum phase transition. The leading instability in the confined phase is an atomic-density wave with subdominant quartet superfluid instability made of four fermions. Finally, we reveal the existence of a bond-ordered Mott insulating phase in some part of the repulsive regime.

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Loading cold atomic gases into optical lattice allows for the realization of bosonic and fermionic lattice models and the experimental study of exotic quantum phases[1]. Ultracold atomic systems also offer an opportunity to investigate the effect of spin degeneracy since the atomic total angular momentum F can be larger than $1/2$ resulting in $2F+1$ hyperfine states. This high-spin physics is expected to stabilize novel exotic phases. In this respect, various superfluid condensates, Mott insulating phases, and interesting vortex structures have been found in spinor bosonic atoms with $F \geq 1$[2,3]. These theoretical predictions might be checked in the context of Bose-Einstein condensates of sodium, rubidium atoms and in spin-3 atom of ^{52}Cr[4]. The spin-degeneracy in fermionic atoms is also expected to give rise to some interesting superfluid and Mott phases. In particular, a molecular superfluid phase might be stabilized where more than two fermions form a bound state. Though such non-trivial superfluid behavior has been previously found in different contexts[5], it has been advocated recently that the formation of bound-state of Cooper pairs is likely to occur in general half-integer $F > 1/2$ ultracold atomic fermionic systems[6,7,8]. In the spin $F = 3/2$ case, it has been predicted on the basis of a low-energy study[6,7] in one dimension that a quartetting superfluid phase, i.e. a bound-state of two Cooper pairs, might be stabilized by strong enough attractive interactions. The simplest lattice Hamiltonian to describe spin-3/2 atoms with s-wave scattering interactions in 1D optical lattice takes the form of a Hubbard-like model[2]:

$$\mathcal{H} = -t \sum_{i,\alpha} \left[c^\dagger_{\alpha,i} c_{\alpha,i+1} + \text{H.c.}\right] + U_0 \sum_i P^\dagger_{00,i} P_{00,i} + U_2 \sum_{i,m} P^\dagger_{2m,i} P_{2m,i}, \quad (1)$$

where $c^\dagger_{\alpha,i}$ is the fermion creation operator corresponding to the four hyperfine states $\alpha = \pm 1/2, \pm 3/2$. The singlet and quintet pairing operators in Eq. (1) are defined through the Clebsch-Gordan coefficient for two indistinguishable particles: $P^\dagger_{JM,i} = \sum_{\alpha\beta} \langle JM|F,F;\alpha\beta\rangle c^\dagger_{\alpha,i} c^\dagger_{\beta,i}$. As it appears, it is more enlightening to express model (1) in terms of the density ($n_i = \sum_\alpha c^\dagger_{\alpha,i} c_{\alpha,i}$) and the singlet pairing operator ($P^\dagger_{00,i} = P^\dagger_i = \frac{1}{\sqrt{2}}[c^\dagger_{\frac{3}{2},i} c^\dagger_{-\frac{3}{2},i} - c^\dagger_{\frac{1}{2},i} c^\dagger_{-\frac{1}{2},i}]$):

$$\mathcal{H} = -t \sum_{i,\alpha} [c^\dagger_{\alpha,i} c_{\alpha,i+1} + \text{H.c.}] + \frac{U}{2} \sum_i n_i^2 + V \sum_i P^\dagger_i P_i, \quad (2)$$

with $U = 2U_2$ and $V = U_0 - U_2$. Model (2) generically displays an exact SO(5) extended spin symmetry and an SU(4) symmetry in the particular case $U_0 = U_2$, i.e. $V = 0$[9]. In sharp contrast with the spin $F = 1/2$ case where both interacting terms in Eq. (2) are proportional, these terms are independent for $F = 3/2$ and strongly compete. While the V-term favors the pairing of two fermions for negative V, an attractive U-interaction might favor the formation of a quartet $Q_i = c_{-\frac{3}{2},i} c_{-\frac{1}{2},i} c_{\frac{1}{2},i} c_{\frac{3}{2},i}$. In fact, it has been recognized in Ref. 6 that the above competition reveals itself through a non-trivial discrete symmetry of the problem. Indeed, model (2) possesses, on top of the SO(5) symmetry, a $\mathbb{Z}_2$ discrete symmetry $\mathcal{U}$: $c_{\alpha,i} \to e^{i\pi/2} c_{\alpha,i}$ which plays a crucial role in the low-energy physics since, as P_i is odd under $\mathcal{U}$, the formation of a quasi-long range BCS phase requires $\mathcal{U}$ to be spontaneously broken. When $\mathcal{U}$ is unbroken the BCS instability is strongly suppressed and the leading superfluid instability is made of four fermions i.e. a quartet which is even under $\mathcal{U}$. Such a two-phase structure has been recently predicted away from half-filling in the weak coupling limit by means of a low-energy approach[6,7,10].

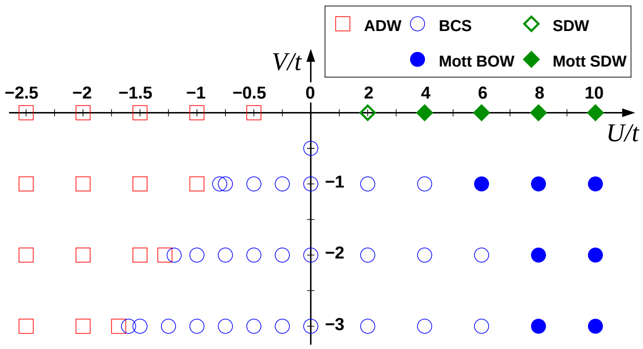

FIG. 1: (Color online) Phase diagram of the spin-3/2 Hubbard chain (2) at quarter filling from QMC and DMRG calculations for $V \leq 0$ (see text for definitions).

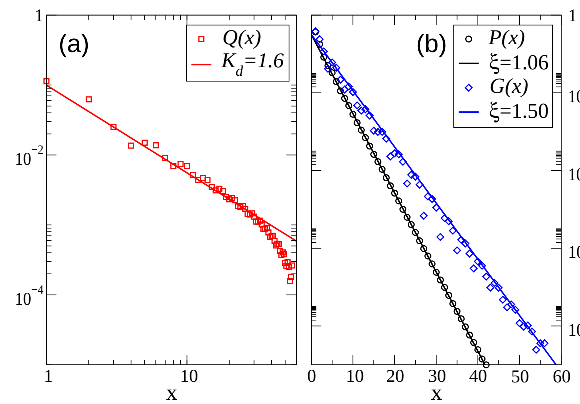

FIG. 2: (Color online) Correlation functions for $U = -1.5t$ and $V = 0$ obtained by DMRG. **(a)** Power-law behavior of the quartet correlations parametrized by Luttinger exponent K_d. **(b)** Short-range behavior of the one-particle Green function and pairing correlations (ξ denotes the correlation lengths).

In this letter, we investigate numerically the phase diagram of model (2) for $V \leq 0$ at quarter filling (one atom per site) by means of quantum Monte-Carlo (QMC) and Density-Matrix Renormalization Group[11] (DMRG) simulations. Physical properties are investigated by computing the one-particle, density, pairing as well as quartetting correlation functions, respectively: $G(x) = \langle c^{\dagger}_{\alpha,i} c_{\alpha,i+x} \rangle$, $N(x) = \langle n_i n_{i+x} \rangle$, $P(x) = \langle P_i P^{\dagger}_{i+x} \rangle$ and $Q(x) = \langle Q_i Q^{\dagger}_{i+x} \rangle$. For the QMC simulations, we used the projector auxiliary field QMC algorithm (see Ref. 12 for the details of the algorithm) in the regime $V \leq 0$ and $U \leq -3V/4$ where the fermionic algorithm has no sign problem[9]. We have studied *periodic* chains with linear size up to $L = 180$ with a typical projection parameter $\Theta t = 10$ and a Trotter time slice $\Delta t = 0.05$. Most of DMRG calculations were performed on *open* chains with $L = 60$ sites and keeping $M = 1400$ states[13]. The resulting phase diagram at quarter filling is presented in Fig. 1 and we now turn to the discussion of the physical properties of the different phases.

Confined Phase – The phase with $U < 0$ and small $|V|$ is characterized by the existence of a spin gap and an unbroken $\mathbb{Z}_2$ discrete symmetry $\mathcal{U}$ which marks the onset of an Atomic Density Wave (ADW) and quartet superfluid quasi-long-range orderings. Indeed, for the typical value of $U = -1.5t$ and $V = 0$, we observe in Fig. 2(b) that both the pairing correlations and the one-particle Green function decay exponentially with distance. In contrast, the quartet correlations are algebraic as it can be seen in Fig. 2(a). We have checked by a direct evaluation that the four-particle gap vanishes. We can thus deduce that the short-range character of $P(x)$ is due to the confinement of Cooper pairs which stems from the unbroken $\mathcal{U}$ symmetry. The above results extend in the whole confined phase (squares in Fig. 1). In this phase, the superfluid instability is of a molecular type made of four fermions: a quartet. However, the density correlations also display a power-law behavior with dominant oscillations at $2k_F = \pi/2$ as it is clearly seen from the Fourier transform $N(q)$ of $N(x)$ presented in

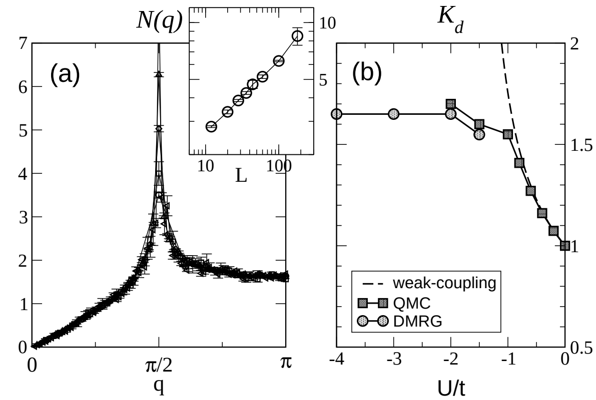

FIG. 3: **(a)** Fourier transform $N(q)$ of the density correlations obtained from QMC ($U = -t$ and $V = 0$). The linear dispersion at small q gives access to the Luttinger parameter K_d. Insert : the scaling of the peak at $2k_F$ vs L signals an ADW phase. **(b)** Luttinger exponent K_d as a function as U.

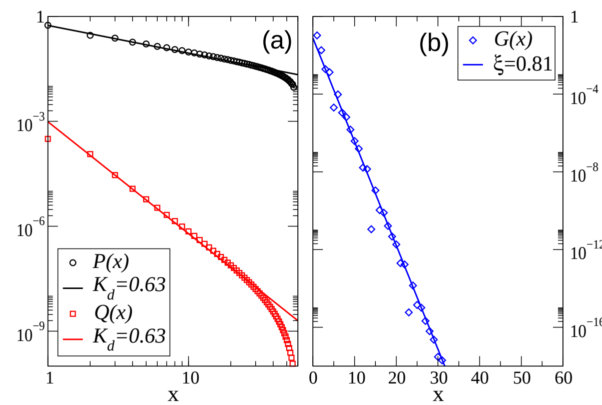

FIG. 4: (Color online) Correlation functions for $U = 0$ and $V = -3t$ from DMRG. **(a)** Pair and quartet correlations are algebraic with $Q(x) \sim P(x)^4$. **(b)** Short-range behavior of the one-particle Green function.

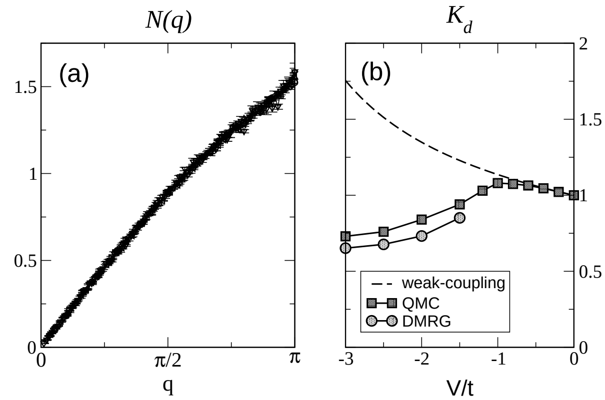

FIG. 5: **(a)** Fourier transform of the density correlations obtained by QMC for $U = 0$ and $V = 1.5t$. **(b)** The Luttinger parameter K_d as a function of V when $U = 0$.

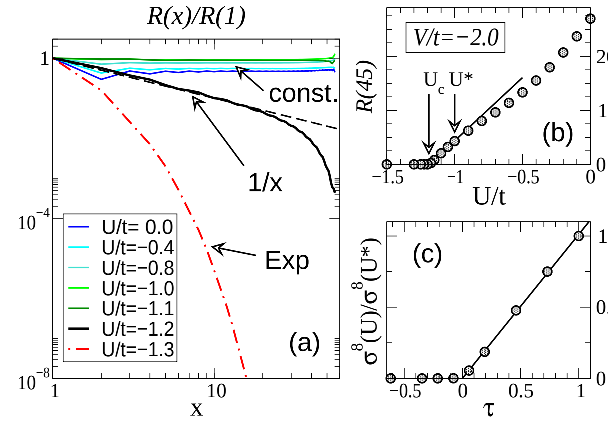

FIG. 6: (Color online) The BCS-ADW transition from DMRG computations along the $V = -2t$ line. **(a)** Normalized ratio $R(x) = P(x)^4/Q(x)$ displaying a critical behavior at the transition. **(b)** In the bulk (at site $x = 45$), $R(x)$ is proportional to $U - U_c$ for $U_c \leq U \leq U^*$ with $U^* = -t$ and $U_c = -1.19t$. **(c)** Plot of $R(U) = \sigma(U)^8$ vs $\tau = (U - U_c)/(U^* - U_c)$ where σ is the Ising order parameter.

Fig. 3(a). The question that naturally arises is which instability dominates in this phase. The answer depends on the value of the non-universal Luttinger parameter K_d which stems from the critical behavior of the density degrees of freedom. Indeed, the quartet and $2k_F$-ADW equal-time correlation functions have been found in Refs.[6,7] to behave at long distance as $Q(x) \sim x^{-2/K_d}$ and $N(x) \sim \cos(\pi x/2)x^{-K_d/2}$. Therefore a quartet superfluid phase with dominant quartet correlations requires $K_d > 2$. The value of K_d has been computed in QMC using the formula:

$$K_d = \frac{\pi}{4} \lim_{q\to 0} \frac{N(q)}{q}, \tag{3}$$

where the factor 4 comes from the four spin states. This procedure has been shown to be very accurate for the spin-1/2 Hubbard model[14]. For DMRG calculations, K_d can be independently obtained from the power-law behavior of the quartet correlations $Q(x)$. Both QMC and DMRG results are shown for example on the SU(4) invariant line ($V = 0$) in Fig. 3(b). We find that QMC works better than DMRG in the weak coupling limit and is in excellent agreement with the perturbative estimate: $K_d^{-2} = 1 + [V + 3U]/(\sqrt{2}\pi t)$[6,7]. For larger $|U|$, DMRG is more accurate and we found that K_d saturates at the value $K_d \simeq 1.6$. Note that the perturbative estimate fails beyond $|U| \geq t$ so that numerical approaches become necessary to estimate K_d. For $V \neq 0$, K_d also saturates at strong couplings to values smaller than 2. We therefore conclude that, though the quartet correlations are quasi-long ranged, the dominant instability in the confined phase is a $2k_F$-ADW.

Deconfined Phase – By allowing V to be sufficiently negative, one can enter a second phase where the one-particle gap is still finite (see Fig. 4(b) for $U = 0, V = -3t$) but the two-particle gap vanishes. In this phase, pairing correlations become algebraic with $P(x) \sim x^{-1/2K_d}$ as shown on Fig. 4(a) and $Q(x)$ remains critical with $Q(x) \sim P(x)^4$ which is the prediction of the low-energy approach. In contrast to the ADW phase, there is no diverging signal at $2k_F = \pi/2$ in $N(q)$ (see Fig. 5(a)). We thus conclude that there is still a spin-gap and the $\mathbb{Z}_2$ symmetry $\mathcal{U}$ is now spontaneously broken which leads to the formation of a quasi-long-range BCS phase. In addition, there is also an ADW instability at $4k_F = \pi$ (see Fig. 5(a) where $N(q)$ has a maximum at $q = \pi$) which has a power-law decay $N(x) \sim \cos(\pi x)x^{-2K_d}$. We thus need to compute numerically K_d to fully characterize the dominant instability of this phase. As in the previous phase, the Luttinger parameter K_d can be extracted either from Eq. (3) (QMC) or from pairing correlations (DMRG). As shown on Fig. 5(b), both results are compatible and agree with the perturbative estimate when $|V| < t$. We find that $K_d > 1/2$ so that the dominant instability in this phase is the BCS singlet pairing.

Quantum phase transition – The striking feature of the phase diagram for attractive U, V interactions is the change of status of the $\mathbb{Z}_2$ symmetry $\mathcal{U}$ which is spontaneously broken (resp. unbroken) in the deconfined (resp. confined) phase. We thus expect a quantum phase transition in the Ising universality class between these two phases. In fact it has been shown in Ref. 6 that the order parameter $\sigma(x)$ associated with the $\mathcal{U}$ symmetry, though being non-local in terms of the lattice fermions, can be extracted from the long-distance behavior of the ratio $R(x) = P(x)^4/Q(x)$. In the confined phase where $\mathcal{U}$ is unbroken, $\langle\sigma(x)\rangle = 0$ and $R(x) \sim \langle\sigma(x)\sigma(0)\rangle^4$ decays exponentially with distance. In the deconfined phase, $\langle\sigma(x)\rangle = \sigma \neq 0$ and $R(x) \sim \sigma^8$. Finally, it has been found in Ref. 6 that at the transition the ratio displays an *universal* power-law behavior: $R(x) \sim 1/x$. We have computed numerically this ratio by DMRG for various parameters to determine the transition line in Fig. 1. The results of Fig. 6(a) clearly show an excellent agreement with the predictions of the low-energy approach.

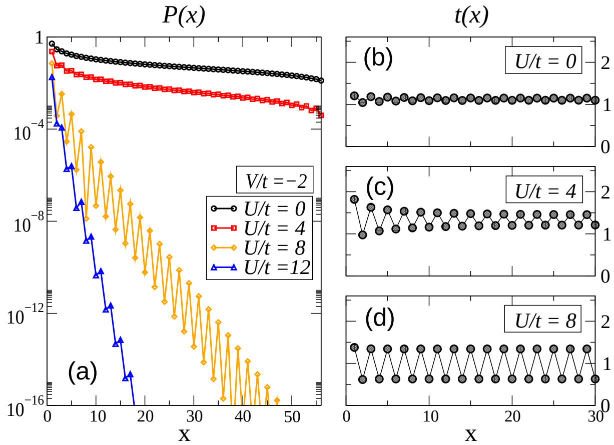

FIG. 7: (Color online) Mott phase for $V < 0$. **(a)** By increasing U, pairing correlations obtained from DMRG change from algebraic to exponential decaying. **(b-d)** The BOW Mott transition is seen from DMRG computations with the appearance of the $4k_F$ order parameter $t(x)$ across the transition.

In particular, we observe that $R(x) \sim 1/x$ near the critical point. In the deconfined phase, $R(x)$ saturates at large distance as it should and is almost independent of x ($R(x) \sim \sigma(U)^8$) when one enters the critical regime (for $U_c \leq U \leq U^*$ in Fig. 6(b)). The plot in Fig. 6(c) demonstrates that $\sigma(U) \sim (U - U_c)^{1/8}$ in full agreement with Ising criticality. In this respect, the situation is in sharp contrast with the $F = 1/2$ well-known case where the $2k_F$-ADW and BCS instabilities coexist for attractive interaction[15].

Mott phase – At quarter-filling, a Mott transition might take place if $K_d < 1/2$ with the formation of a density gap[6,7]. For the repulsive SU(4) Hubbard chain ($V = 0$), the QMC study of Ref. 16 found a transition from a gapless spin-density wave (SDW) to a generalized Mott SDW with three gapless spin modes (see Fig. 1). For $V < 0$, we expect an entirely different Mott phase due to the presence of a spin gap and the breaking of the $\mathbb{Z}_2$ symmetry $\mathcal{U}$. In the Mott region in Fig. 1 (full circles), the BCS singlet pairing becomes short-ranged as shown in Fig. 7(a) and we find that, as the density gap opens, the local density almost does not fluctuate and $N(x) \sim 1$. In contrast, the local kinetic bond, $t(x) = \langle \sum_\alpha c^\dagger_{\alpha,x+1} c_{\alpha,x} + \text{H.c.}\rangle$, orders with a $4k_F = \pi$ modulation reminiscent of a *doubly* degenerate ground state as it can be seen in Fig. 7(b-d) for $V = -2t$. We therefore conclude on the emergence of a bond-ordering Mott phase with periodicity two (Mott BOW in Fig. 1).

Concluding remarks – We conclude this letter in emphasizing that the existence of a quartet superfluid phase where quartet correlations dominate over the $2k_F$-ADW instability relies on the non-universal Luttinger parameter K_d. Though $K_d < 2$ at *quarter* filling, we expect that at sufficiently low densities, K_d may become larger than 2, which marks the onset of the quartetting phase. The formation of this exotic phase will be discussed in a forthcoming paper.

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